Assistant Professor

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Fundamental Insights about Geochemical Surface Science from Density Functional Theory

Research interests: developing the fundamental understanding of metal (hydr)oxide reactivity. Currently, focusing on two categories of model systems: Giant aluminum polycations (GAPs) and Periodic Slab Models (PSMs).

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Abstract
Adsorption processes of ionic species on the surfaces of naturally occurring metal hydroxides influence aqueous contaminant transport and fate, and are also fundamentally related to technological applications such as batteries and heterogeneous catalysis. Essential chemical information about environmental interface structure-reactivity relationships is becoming accessible through quantum mechanical modeling. Computational studies provide a perfectly controllable, safe, and affordable means to interpret experimental information, to predict properties that cannot be measured, and to develop conceptual, molecular-level understanding of these systems. While the ability of metal hydroxide surfaces to bind contaminants has been established, identification of the specific reactivity factors and a mechanistic understanding of the adsorption process is lacking. We highlight how we use our DFT studies to extract new chemical understanding of the surface and particle properties that dictate reactivity and discuss ongoing work and future goals, including issues of DFT accuracy and towards the development of new conceptual models. Long-term goals include harnessing our new molecular-level understanding of environmental surfaces towards the rational design of engineered sorbents.